I U C L I D
Data Set

Existing Chemical ID:	3618-72-2
CAS No.	3618-72-2
Product name	C.I. Disperse Blue 79:1
Colour index number	11344
CAS Name	Acetamide, N-[5-[bis[2-(acetyloxy)ethyl]amino]-2-[(2-bromo-4,6-dinitrophenyl)azo]-4-methoxyphenyl]-
EINECS No.	222-813-1
Molecular Formula	C23H25BrN6O10
Creation date:	27-FEB-2001
Consortium:	ETAD North America Disperse Blue 79:1 Coalition
Number of Pages:	24

Company Information

1.0.1 OECD and Company Information

Type: lead organization
Name: ETAD North America Disperse Blue 79:1 Coalition
Street: 1850 M Street, NW, Suite 700
City/State: Washington, DC
Zip Code: 20036
Country: United States
Phone: 202-721-4100
Telefax: 202-296-8120
Remark: Dr. C. T. Helmes - contact

Type: cooperating company
Name: Blackman Uhler Chemical Company
Street: PO Box 5627
City/State: Spartanburg, SC
Zip Code: 29304
Country: United States
Phone: 864-585-3661
Telefax: 864-596-1501
Remark: Bert Moore - Contact

Type: cooperating company
Name: Ciba Specialty Chemicals Corporation
Street: PO Box 2444
City/State: High Point NC
Zip Code: 27261-2493
Country: United States
Phone: 336-801-2618

Telefax: 336-801-3077
Remark: Tom Dukes - Contact

Type: cooperating company
Name: Clariant Corporation
Street: 4000 Monroe Road
City/State: Charlotte NC
Zip Code: 28205
Country: United States
Phone: 704-331-7719
Telefax: 704-331-7718
Remark: Carole Dixon - contact

Type: cooperating company
Name: DyStar L.P.
Street: 9844-A Southern Pine Boulevard
City/State: Charlotte NC
Zip Code: 28273
Country: United States
Phone: 704-561-2644
Telefax: 704-561-3098
Remark: Will Caylor - contact

GENERAL SUBSTANCE INFORMATION

1.1 General Substance Information

A. TYPE OF SUBSTANCE

element [ ]; inorganic [ ]; natural substance [ ];
organic [**X**]; organometallic [ ]; petroleum product [ ]
Reference: (19)

B. PHYSICAL STATE

gaseous [ ]; liquid [ ]; solid [**X**]
Reference: (19)

C. PURITY

>97% based on High Performance Liquid Chromotography (HPLC)
Reference: (19)

PHYSICAL CHEMICAL PROPERTIES

2.1 Melting Point

Value: >= 138 degree C
Year: 1989
GLP: no data
Test substance: Foron Navy S-2GRL Purified Presscake
(i.e., C.I. Disperse Blue 79:1)
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint

Reference: (9)

2.2 Boiling Point

Value: = 476 degree C
Year: 1996
GLP: no data
Test substance: C.I. Disperse Blue 79 (CAS No. 12239-34-8)
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
Reference: (16)

2.4 Vapour Pressure

Value: = 4.53 x 10^{-9} hPa at 25 degree C
Year: 1996
GLP: no data
Test substance: C.I. Disperse Blue 79 (CAS No. 12239-34-8)
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
Reference: (16)

2.5 Partition Coefficient

log Pow: = 4.44 at 25 degree C
method: measured
Year: 1999
GLP: no data
Method: Disperse Blue 79:1 was first recrystallized in dichloromethane to remove any additives prior to use. In a 1-L thermostated flask, 800 ml of distilled water and 100 ml of octanol were added and slowly stirred with 0.4 9/L test substance at 25 degrees Celsius. The dye was dissolved in octanol, then the required amount of octanol was pipetted off and flushed gently into the thermostated flask on top of the water. During a three week period, several samples of water and octanol were taken and the concentration of the dye was determined in both solutions. The Kow was determined from the ratio of the concentrations in octanol and water, respectively, at equilibrium. Each measurement was performed in triplicate thermostated flasks.

Test substance: C.I Disperse Blue 79:1 was first recrystallized in dichloromethane to remove additives prior to use.

Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment.

Flag: Critical study for SIDS endpoint

Reference: (10)

2.6.1 Water Solubility

Value: = 0.0052 mg/1 at 25 degree C
Description: of low solubility
Year: 1989
GLP: no data
Method: Generator column technique. The generator column contained 100-120 mesh XAD-2 resin on which the dye had been coated. The resin was coated by adding 0.03 g of dye to several millimeters of acetonitrile in a 50 mL round bottom flask before the addition of 1.3 g of resin.

A 0.25 X 10 stainless steel column fitted with a 0.5 micrometer exit and 1.0 micrometer inlet frit was dry packed with the resin and dye material.

Unbuffered distilled water was pumped through the columns at a flow rate of 0.1 to 2.0 mL per minute. Before taking the first samples, at least one liter of water was pumped through the column.

The concentrator column was a 30 X 0.8cm pyrex tube containing a 5 cm section XAD-2 resin with containment plugs of glass wool on either side. After water had been allowed to flow through the generator and concentrator columns, the concentrator column was eluted with 2-3 mL of acetonitrile into a tared 20 mL vial.

Quantitation was performed by HPLC using Kratos Model 400 pump acetonitrile/water at a flow rate of 1.3 mL per minute.

Test substance: C.I. Disperse Blue 79:1

Reliability: (1) valid without restrictions
Meets generally accepted scientific method and is described in sufficient detail.

Flag: Critical study for SIDS endpoint

Reference: (1)

ENVIRONMENTAL FATE AND PATHWAYS

3.1.1 Photodegradation

Type: Air
INDIRECT PHOTOLYSIS
Sensitizer: OH
Conc. of sens.: 1.5×10^{6} OH/cm^3
Rate constant: 226.06×10^{-12} cm^3/molecule-sec
Degradation: 50% after 0.568 hours
Method: other (calculated): AOP Program (v1.90)
GLP: no
Test substance: C.I. Disperse Blue 79:1
Reliability: (2) valid with restrictions; accepted calculation method
Flag: Critical study for SIDS endpoint
Reference: (17)

3.1.2 Stability in Water

Type:	biotic
$t_{1/2}$ pH 6. 8:	<= 4 hour
Deg. Product:	yes
Year:	1995
GLP:	no data
Method:	Disperse Blue 79:1 was reduced in three, high organic carbon content anoxic sediment-water systems.
Result:	The half-life ranged from 40 minutes to 4 hours. The reaction pathway for the sediment-mediated reduction of Disperse Blue 79:1 resulted principally in the formation of a N,N-disubstituted 1,4-diaminobenzene, 3-bromo-6-nitro-1, 2-diaminobenzene, and a benzimidazole.
Test substance:	C.I. Disperse Blue 79:1
Conclusion:	Results of this study suggest that Disperse Blue 79:1 can undergo rapid reductive transformation in anoxic bottom sediments, resulting in the release of aromatic amines to the water column.
Reliability:	(2) valid with restrictions Accepted calculation method.
Flag:	Critical study for SIDS endpoint
Reference:	(14)

3.3.1 Transport between Environmental Compartments

A. ADSORPTION

Type:	adsorption
Media:	water - soil
Year:	1989
GLP:	no data
Method:	Water solubilities and octanol/water partition coefficients were used to predict expected concentration factors for sediment and biota.
Result:	The results show that Disperse Blue 79:1 has a potential toward sediment sorption and bioconcentration. Measured water solubility was 5.2 ug/l. The calculated LogKp (sediment concentration factor) was 3.9 and the calculated LogBCF (bioconentration factor) was 4.1. The log of the measured partition coefficient (octanol/water) was 4.8.
Test substance:	C.I. Disperse Blue 79:1
Conclusion:	Available data from this study suggest that Disperse Blue 79:1 is likely to accumulate extensively in sediment and biota.

Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment.

Flag: Critical study for SIDS endpoint

Reference: (15)

B. FUGACITY MODEL LEVEL III
Type: fugacity model level III
Media: other: air-water-soil-sediment
Year: 2001
GLP: no data
Method: other: EPIWIN modeling program

Result: Chemical Name: C.I. Disperse Blue 79:1
Molecular Weight:625.39
Henry's LC: 9.82e-025 atm-m3/mole (Henrywin program)
Vapor Pressure: 1.74e-017 mm Hg (Mpbpwin program)
LogKow: 4.8 (Kowwin program)
Soil Koc: 2.59e+004 (calc by model)

	Concentration (percent)	Half-life (hr)	Emissions (kg/hr)	Fugacity (atm)
Air	2.13e-101	1.14	1000	1.57e-028
Water	6.69	3.6e+003	1000	6.24e-030
Soil	79.4	3.6e+003	1000	1.38e-030
Sediment	13.9	1.44e+004	0	1.08e-029

	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.61e-005	2.63e-007	5.36e-007	8.87e-009
Water	159	828	5.32	27.6
Soil	1.9e+003	0	63.2	0
Sediment	82.7	3.34	2.76	1.15

Persistence Time: 4.13e+003 hr
Reaction Time: 5.8e+003 hr
Advection Time: 1.44e+004 hr
Percent Reacted: 71.2
Percent Advected: 28.8

Test substance: C.I. Disperse Blue 79:1

Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment.

Flag: Critical study for SIDS endpoint

Reference: (17)

B. FUGACITY MODEL LEVEL III

Type: fugacity model level III
Media: other: air-water-soil-sediment
Year: 2001
GLP: no data
Method: other: EPIWIN modeling program

Result: Chemical Name: C.I. Disperse Blue 79
Molecular Weight:639.42
Henry's LC: 1.3e-024 atm-m3/mole (Henrywin program)
Vapor Pressure: 7.2e-018 mm Hg (Mpbpwin program)
LogKow: 5.53 (Kowwin program)
Soil Koc: 1.39e+005 (calc by model)

	Concentration (percent)	Half-life (hr)	Emissions (kg/hr)	Fugacity (atm)
Air	4.6e-101	1.73	1000	2.03e-028
Water	3.68	3.6e+003	1000	4.95e-030
Soil	60.9	3.6e+003	1000	3.34e-031
Sediment	35.4	1.44e+004	0	8.74e-030

	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	2.99e-055	7.45e-007	9.97e-007	2.48e-008
Water	115	596	3.83	19.9
Soil	1.9e+003	0	63.3	0
Sediment	276	115	9.2	3.82

Persistence Time: 5.4e+003 hr
Reaction Time: 7.07e+003 hr
Advection Time: 2.28e+004 hr
Percent Reacted: 76.3
Percent Advected: 23.7

Test substance: C.I. Disperse Blue 79

Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment.

Flag: Critical study for SIDS endpoint

Reference: (17)

3.5 Biodegradation

A. ANAEROBIC DEGRADATION STUDY 1

Type: aerobic and anaerobic
Inoculum: activated sludge
Contact time: 5 day
Result: other: degraded under anaerobic conditions
Deg. Product: not measured
Year: 1995
GLP: no data
Method: This study, conducted by EPA, was done to determine the effectiveness of a wastewater treatment plant from a

Disperse Blue 79:1 production facility in the removal of dye from a waste stream.
Grab samples were collected from the effluent of a production plant, the bottom of a secondary clarifier and the effluent of a waste treatment plant (WTP) over a period of five days.

Result: The highest concentrations of Disperse Blue 79:1 were found in the samples collected from the bottom of the secondary clarifier. Significant reduction (90%) of the dye concentration was observed in the WTP effluent (e.g. 116 mg/kg) compared to the WTP influent (e.g. 1,714 mg/kg) over the five day period.

No degradation of the dye was observed in the waste stream or WTP of the production plant. No Disperse Blue 79:1 was detected in the sediment or water samples downstream of the point where treated effluent enters the river.

Test substance: C.I. Disperse Blue 79:1

Conclusion: The results suggest that the primary dye removal process occurs in the settling of particulate matter in the primary and secondary clarifiers. Most of the dye is removed from the WTP by the settling of this particulate matter and adsorption on to activated sludge.

Accumulation in the bottom sediments does not occur, as shown in the sediment and water samples taken downstream of the production plant WTP.

Complete removal of Disperse Blue 79:1 from the Plant effluent occurred through degradation under anaerobic conditions.

Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment

Flag: Critical study for SIDS endpoint

Reference: (8)

B. ANAEROBIC DEGRADATION STUDY 2

Type: aerobic and anaerobic
Inoculum: Activated Sludge from the Milwaukee Metropolitan Sewerage District South Shore Wastewater Treatment Plant
Concentration: 443 mg/l related to Test substance
7.86 mg/l related to Test substance
Contact time: 15 day
Degradation: = 98.2% after 15 day
Year: 1989
GLP: no data
Method: EPA Study; Degradation via anaerobic digester

Result: A 98% reduction in the average concentration of dye in the final effluent was observed.

Test substance: C.I. Disperse Blue 79:1

Conclusion: The majority of the Disperse Blue 79:1 fed to an activated sludge system was removed in the waste activated sludge.

Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment

Flag: Critical study for SIDS endpoint

Reference: (7)

ECOTOXICITY ELEMENTS

Aquatic Organisms

4.1 Acute/Prolonged Toxicity to Fish

See section 4.5.1.

4.2 Acute Toxicity to Aquatic Invertebrates

Species: Daphnia magna (Crustacea)
Exposure Period: 24 hours
Unit: mg/l
Analytical Monitoring: no data
EC0: =1.6
EC50: =16
EC100: >50
Method: OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year: 1984
GLP: yes
Test Substance: C.I. Disperse Blue 79 (CAS No. 12239-34-8)
Remark: Results are given in mg (active substance)/1.

Reliability: (1) valid without restriction
Comparable to guideline study

Flag: Critical study for SIDS endpoint

Reference: (4)

4.3 Toxicity to Aquatic Plants e.g., Algae

A. BIOMASS
Species: Scenedesmus subspicatus (Algae)
Endpoint: biomass
Exposure Period: 72 hours

Unit: mg/l
Analytical Monitoring: no data
EC10: = 2.9
EC50: = 15
Method: OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year: 1984
GLP: yes
Test Substance: C.I. Disperse Blue 79 (CAS No. 12239-34-8)
Remark: Results are given in mg (active substance)/l.

Reliability: (1) valid without restriction
Comparable to guideline study

Flag: Critical study for SIDS endpoint

Reference: (4)

B. GROWTH RATE
Species: Scenedesmus subspicatus (Algae)
Endpoint: growth rate
Exposure Period: 72 hours
Unit: mg/l
Analytical Monitoring: no data
NOEC: = 2
EC10: = 3
EC50: = 9.5
Method: OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year: 1984
GLP: yes
Test Substance: C.I. Disperse Blue 79 (CAS No. 12239-34-8)
Remark: Results are given in mg (active substance)/l.

Reliability: (1) valid without restriction
Comparable to guideline study.

Flag: Critical study for SIDS endpoint

Reference: (4)

4.5.1 Acute/Chronic Toxicity to Fish

Species: Oncorhynchus mykiss (Fish, fresh water)
Endpoint: length, weight, reproduction rate, survival
Exposure period: 122 day
Unit: µg/l Analytical monitoring: yes
NOEC: >= 4.8
Year: 1991
GLP: yes
Method: An early life stage toxicity study of test substance C.I. Disperse Blue 79:1 in Rainbow Trout using a flow-through system was completed in 1991 at ABC Laboratories, Inc., Columbia, MO.

Newly fertilized eggs (fertilized < 4 hours before study initiation) were used for the initiation of the study with exposure continuing for 122 days post-hatch. A 2-liter proportional diluter system was used to maintain constant test concentrations. Exposure concentrations of test substance were determined by spectrophotometric analysis.

The test system dilution water consisted of deep well water which had been passed through a reverse osmosis system then blended back with additional well water to a total hardness of approximately 160-180 mg/l (as $CaC0_3$)and a pH of approximately 8.3. The water temperature was maintained at 10 +/- 1.5 degrees C during egg incubation and 12 +/- 1.5 degrees C during fry growth. The flow rate was 303 L/day initially and increased to 572 L/day during the final two weeks of the study.

The mean measured concentrations of test substance were 0.36, 0.58, 1.2, 2.5, and 4.8 µg/l. These values ranged from 92% to 116% of the nominal test concentrations of 0.31, 0.63, 1.3, 2.5, and 5.0 µg/l. The high nominal test concentration of 5.0 µg/l was considered to be the limit of solubility for the test substance.

Result: The Maximum Acceptable Toxicant Concentration (MATC) Limits, which consists of the no-observed effect concentrations (NOEC) and the lowest observed effect concentration (LOEC), is based on the statistically analyzed parameters of hatchability, survival, and fry growth (length and weight). No statistically significant reductions in hatchability were detected at any test concentration. Fry survival was analyzed at four intervals: 20, 60, 90, 122 days post-hatch. No statistically significant survival reductions were indicated at any test level for either the 20 or 60 day post hatch intervals. Marginally significant reductions in survival were detected at 2.5 µg/l for both the 90 and 122 day post-hatch intervals, but these reductions were not considered to be concentration-related or biologically significant. Therefore, the 2.5 µg/l dose was not considered as an effect level with regard to survival. Length was not significantly reduced at any test level when measured at 60, 90, 122 days post-hatch. At study termination (122 days post-hatch), weight was not significantly reduced at any test level.

Test Substance: C.I. Disperse Blue 79:1 Purified Presscake, Lot Number KA0008, BRRC Sample Number 53-10. Green powder at room temperature, >97% pure.

Conclusion: Based on the results from this study, the NOEC was determined to be greater than or equal to the highest measured test concentration of 4.8 µg/l. This measured test concentration was based on the highest nominal test level of 5.0 µg/l, which is considered to be the limit of water solubility. No LOEC could be determined because there were no concentration-related effect levels. Therefore, a point

estimate MATC value (i.e., the geometric mean of the NOEC and the LOEC) could not be calculated. [ABC Laboratories, Inc., 1991]
The U.S. Environmental Protection Agency has concluded that the ecological risks of C.I. Disperse Blue 79:1 are expected to be low, based on the low toxicity observed at its water solubility (equal to or greater than 4.8 µg/l). [EPA, 1993]

Reliability: (1) valid without restriction
Valid without restriction.
Meets national standards method. U.S. E.P.A., 40 CFR 797.1600 Fish Early Life Stage Toxicity Test with Modification.

Flag: Critical study for SIDS endpoint

Reference: (2)(3)

HEALTH ELEMENTS

5.1.1 Acute Oral Toxicity

Type: 14-Day Range Finding for 90-Day Subchronic Toxicity
Species: rat
Strain: Sprague-Dawley
Sex: male/female
Number of Animals: 5
Vehicle: corn oil
Value: = 2500 mg/kg bw
Year: 1991
GLP: yes
Method: Study conducted to comply with GLP regulations, TSCA, and 40 CFR part 793.

Male and female rats (5 per group) were administered the test substance by oral gavage at concentrations of 0, 100, 500, 1000, or 2500 mg/kg/day 5 days per week for 2 weeks plus an additional dose on the following Monday (11 doses).

Result: No treatment-related effects on daily clinical signs, body weights, body weight gains, food consumption, and necropsy were observed at any dose level.

Test substance: C.I. Disperse Blue 79:1 Purified Presscake, Lot Number KA0008, BRRC Sample Number 53-10. Green powder at room temperature, >97% pure.

Conclusion: Based on the lack of evidence of treatment-related effects, it was concluded that a dose of 2500 mg/kg/day is the maximum amount of C.I.Disperse Blue 79:1 that can be administered to rats on a continuous basis.

Reliability: (1) valid without restriction
GLP guideline study; 40 CFR Part 793

Flag: Critical study for SIDS endpoint

Reference: (3)(13)

5.4 Repeated Dose Toxicity

Species: rat
Sex: male/female
Strain: Sprague-Dawley
Route of admin.: gavage
Exposure period: 90 days
Frequency of treatment: 5 days per week
Doses: 250, 1250, 2500 mg/kg bw/day
Control Group: yes, concurrent vehicle
NOAEL: = 2500 mg/kg
Year: 1991
GLP: yes
Method: Dosing suspensions were prepared at concentrations of 5, 125 and 250 mg/ml of corn oil. Corn oil was used in dosing the control animals. Doses were administered as suspensions in corn oil at a volume of 10 ml/kg/day by gavage five days per week over a period of 13 weeks.

Observations and measurements included mortality, clinical signs, body weights, body weight gains, food consumption, ophthalmic examinations, organ weights, hematology, clinical chemistry, gross pathology and histopathology.

After week 13, the rats were anesthetized and sacrificed.

Result: Blue coloration of the body and/or tail was observed in some of the animals from all dose groups of male animals and one female from each of the mid and high dose groups. This coloration is not considered biologically significant since the test substance is a dye with an intense blue color. No other treatment-related observations were made for any group treated with Disperse Blue 79:1.

There were no treatment-related differences in food consumption, body weights, ophthalmic examinations, clinical pathology, organ weights, final body weights, necropsy or histopathology observations in those animals treated with Disperse Blue 79:1.

Test Substance: C.I. Disperse Blue 79:1 Purified Presscake, Lot Number KA0008, BRRC Sample Number 53-10. Green powder at room temperature, >97% pure.

Conclusion: C.I. Disperse Blue 79:1 did not result in any toxicity when administered by gavage to Sprague-Dawley rats 5 days per week for 13 weeks at levels as high as 2500 mg/kg/day. Higher dosing levels were precluded due to limitations of

the amount of test substance that could be suspended in corn oil and the amount of corn oil that could be administered to rats in one day.
The blue coloration observed in hair, tails, urine and fecal material of some of the animals can be attributed to the intense blue color of the test substance.

The NOEL for Disperse Blue 79:1 in Sprague Dawley rats under the conditions of this study was at least 2500 mg/kg/day.

Reliability: (1) valid without restriction
Meets generally accepted scientific method and is described in sufficient detail.

Flag: Critical study for SIDS endpoint

Reference: (3) (13)

5.5 Genetic Toxicity In Vitro

A. BACTERIAL TEST
Type: Ames *S. typhimurium* bacterial mutagenicity assay.
System of testing: *S. typhimurium* strains TA1537, TA1538, TA98, and TA100
Concentration: 1 to 1,000 µg/plate
Metabolic activation: With **[ ]**; Without **[ ]**; With and Without **[X]**; No data **[ ]**
Results:
Genotoxic effects: Positive
GLP: no data
Method: The mutagenicity of the test substance was determined using the Ames *S. typhimurium* bacterial mutagenicity assay. Experimental results were evaluated by comparing the number of histidine-independent colonies on treated agar plates with control plates. Mutagenicity was established by demonstration of a mutagenic dose-response relationship.

The test chemical was assayed at a dose range of 1 to 1,000 µg/plate, both with and without metabolic activation, in *S. typhimurium* strains TA 1537, TA1538, TA98, and TA100 obtained from Dr. Bruce Ames of the University of California at Berkeley. Metabolic activation was achieved by an Aroclor 1254-stimulated rat liver system.

The test article was serially diluted in DMSO and added at a volume of 0.05 ml to the plate incorporation assay consisting of 2.00 ml of an agar medium, 0.05 ml of the indicator organisms (about 10^8 bacteria), and 0.50 ml of the metabolic activation mixture (if appropriate). Plates were incubated for 48 hours at 37° C, after which revertent colonies were counted using a BioTran II automated colony counter when possible or manually with an electric probe colony counter when precipitation precluded automatic

counting. All assays were repeated at least once on a separate day.

Test substance: Foron Navy SE-2GRL, purity: no data
Remarks: Under conditions of the test, it was concluded that the test substance is mutagenic in *S. typhimurium* strains TA1537, TA1538, TA98,and TA100.

Reliability: (1) valid without restriction
Meets generally accepted scientific data.

Flag: Critical study for SIDS endpoint

Reference: (18)

B. NON-BACTERIAL IN VITRO TEST
Type: Mammalian cell gene mutation assay
System of testing: Mammalian cell V79
Concentration: Without metabolic activation: 0.05 to 1.0 µg/ml; with 2.5 to 750 µg/ml
Metabolic activation: With **[ ]**; Without **[ ]**; With and Without **[X]**; No data **[ ]**
Results: NEGATIVE
GLP: Yes
Method: Other

Test substance: C.I. Disperse Blue 79 (CAS 12239-34-8), purity: no data

Remarks: The substance was non-genotoxic under conditions of test.

Reliability: (1) valid without restriction
Meets generally accepted scientific data.

Flag: Critical study for SIDS endpoint

Reference: (16)

5.6 Genetic Toxicity In Vivo

A. MICRONUCLEUS ASSAY
Type: Micronucleus assay
Species/strain: Mouse/NMRI
Sex: Male/Female
Route of Admin.: Gavage
Exposure period: No data
Doses: 5,000 mg/kg
Results: No induction of chromosome mutations.
Genotoxic effects: Not considered mutagenic
Method: OECD Guideline 474: "Genetic Toxicology: Micronucleus Test." (1983)
GLP: Yes
Test substance: C.I. Disperse Blue 79 (CAS 12239-34-8), purity: no data

Reliability: (1) valid without restriction
Meets generally accepted scientific method and is described in sufficient detail.
Flag: Critical study for SIDS endpoint

Reference: (16)

B. DROSOPHILA SLRL TEST
Type: Drosophila SLRL test
Species: Drosophila melanogaster
Sex: male/female
Strain: other: Canton-S Wild Type stock
Route of admin.: s.c.
Exposure period: Administration of the chemical was by injection to 2-3 day old males, who were mated to untreated females. F-1 females were mated individually to brothers. Running time was 19-21 weeks.
Doses: 50 ppm
Result: negative
Year: 1990
GLP: yes
Method: The chemical C.I. Disperse Blue 79:1 was tested for mutagenic activity (the induction of sex-linked recessive lethal mutations) in Drosophila melanogaster adult males exposed by injection.

The males were injected with approximately 0.3 µl of the test material at a concentration of 50 ppm in 1.9% DMSO and 0.1% Tween 80 carried in 0.7% aqueous saline. This combination of solvents was chosen based on the limited solubility of the test chemical. The material was not toxic at this concentration and no male sterility was induced.

A standard genetic scheme (Basc females crossed with Canton-S wild type males) was employed and post-meiotic germ cells at the time of exposure were tested for lethal mutations.

Result: The sex-linked recessive lethal results (shown below) show no difference between treated samples and negative controls. All frequencies are well within the laboratory's range of recent historical control values:

DB 79:1, 50 ppm	17/14740	(0.115%)
negative control	16/14416	(0.111%)
DMN 500 ppm (positive control)	58/1208	(4.801%)

Test substance: C.I. Disperse Blue 79:1 Purified Presscake, Lot Number KA0008, BRRC Sample Number 53-10. Green powder at room temperature, >97% pure.

Conclusion: It is concluded that C.I. Disperse Blue 79:1 does not induce mutations in the post-meiotic germ cells of Drosophila melanogaster when administered by injection to adult males.

Reliability: (1) valid without restriction
Meets national standards method. EPA OPPTS 870.5275

Flag: Critical study for SIDS endpoint

Reference: (3)(5)

5.8 Reproductive Toxicity

Species: rat
Sex: male/female
Strain: Sprague-Dawley
Route of admin.: gavage
Exposure period: 90 days
Frequency of treatment: 5 days per week
Doses: 250, 1250, 2500 mg/kg bw/day
Control Group: yes, concurrent vehicle
NOAEL: = 2500 mg/kg
Year: 1991
GLP: yes
Method: Dosing suspensions were prepared at concentrations of 5, 125 and 250 mg/ml of corn oil. Corn oil was used in dosing the control animals. Doses were administered as suspensions in corn oil at a volume of 10 ml/kg/day by gavage five days per week over a period of 13 weeks.

Observations and measurements included mortality, clinical signs, body weights, body weight gains, food consumption, ophthalmic examinations, organ weights, hematology, clinical chemistry, gross pathology and histopathology.

After week 13, the rats were anesthetized and sacrificed.

Result: Blue coloration of the body and/or tail was observed in some of the animals from all dose groups of male animals and one female from each of the mid and high dose groups. This coloration is not considered biologically significant since the test substance is a dye with an intense blue color. No other treatment-related observations were made for any group treated with Disperse Blue 79:1.

A complete necropsy was performed on each animal, including those that died during the study. Histology was performed on all tissues including reproductive organs from each dosing group and the control group. There were no gross or microscopic lesions attributed to treatment with Disperse Blue 79:1 for either sex at any dose level.

Test Substance: C.I. Disperse Blue 79:1 Purified Presscake, Lot Number KA0008, BRRC Sample Number 53-10. Green powder at room temperature, >97% pure.

Conclusion: C.I. Disperse Blue 79:1 did not result in any reproductive toxicity when administered by gavage to Sprague-Dawley rats 5 days per week for 13 weeks at levels as high as 2500 mg/kg/day. Higher dosing levels were precluded due to limitations of the amount of test substance that could be suspended in corn oil and the amount of corn oil that could be administered to rats in one day.
The blue coloration observed in hair, tails, urine and fecal material of some of the animals can be attributed to the intense blue color of the test substance.

The NOEL for Disperse Blue 79:1 in Sprague Dawley rats under the conditions of this study was at least 2500 mg/kg/day.

Reliability: (1) valid without restriction
Meets generally accepted scientific method and is described in sufficient detail.

Flag: Critical study for SIDS endpoint

Reference: (3) (13)

5.9 Developmental Toxicity/Teratogenicity

A. RAT
Species: rat
Sex: female
Strain: Sprague-Dawley
Route of admin.: gavage
Exposure period: Days 6 through 15 of gestation
Frequency of treatment: Once daily
Duration of test: 20 days
Doses: 0, 500, 1000, or 2000 mg/kg/day in corn oil.
Control Group: yes, concurrent vehicle
NOAEL Maternalt.: = 2000 mg/kg bw
NOAEL Teratogen.: = 2000 mg/kg bw
Year: 1990
GLP: yes
Method: Pregnant Sprague-Dawley rats were exposed by gavage to C.I. Disperse Blue 79:1 once daily on days 6 through 15 of gestation.

Result: At scheduled sacrifice on gestational day 20, maternal body weights and weight gains were equivalent for all groups for all time points. No maternal clinical signs appeared to be treatment related except for green, dark and/or dark green feces in the treated groups. Maternal food consumption showed no treatment related differences and all gestational parameters were equivalent across all groups including pre and postimplantation loss and fetal body weights/litter. There were no treatment related increased incidences in individual or pooled external, visceral, skeletal or total fetal malformations or variations.

Test substance: C.I. Disperse Blue 79:1 Purified Presscake, Lot Number KA0008, BRRC Sample Number 53-10. Green powder at room temperature, >97% pure.

Conclusion: In conclusion, C.I. Disperse Blue 79:1 administered by gavage during major organogenesis in Sprague-Dawley rats resulted in no maternal or developmental toxicity at any dose tested. The "no observable adverse effect level" (NOAEL) for maternal and developmental toxicity of C.I. Disperse Blue 79:1 in rats is therefore at least 2000 mg/kg/day under the conditions of this study.

Reliability: (1) valid without restriction
GLP guideline study.

Flag: Critical study for SIDS endpoint

Reference: (3)(11)

B. RABBIT

Species: rabbit
Sex: female
Strain: New Zealand white
Route of admin.: gavage
Exposure period: 13 days (gestational days 6-18)
Frequency of treatment: once daily
Duration of test: 30 days
Doses: 0, 100, 300, 600 mg/kg/day
Control Group: yes, concurrent vehicle
NOAEL Maternalt.: = 100 mg/kg bw
NOAEL Teratogen.: = 300 mg/kg bw
Year: 1991
GLP: yes
Method: Artificially inseminated New Zealand White rabbits, 16 females per group, were exposed to test substance by gavage once daily on gestational days 6 through 18 at doses of 0, 100, 300, or 600 mg/kg/day in corn oil. Clinical observations were taken daily and maternal body weights were taken at regular intervals from gestational days 0 through 30.

At scheduled sacrifice on gestational day 30, the does were subjected to a gross necropsy and full examination.

Result: Maternal body weights and weight changes were statistically equivalent across all groups, for all intervals evaluated, but maternal gestational weight change was clearly reduced at the 300 and 600 mg/kg/day dose levels. Gravid uterine and liver weights were unaffected by treatment. Food consumption was equivalent across all doses for all intervals except for a significant increase at 600 mg/kg/day for gestational days 6 through 9.

Gestational parameters, including pre- and postimplantaton loss and fetal body weights per litter, were statistically equivalent across all groups. A slight but not statistically significant reduction in fetal body weights per litter (all fetuses and males, but not females) was observed at 600 mg/kg/day, unaccompanied by any other indications of developmental toxicity. Also, no treatment-related increased incidences of individual or pooled external, visceral, skeletal or total fetal malformations or variations were observed.

Test substance: C.I. Disperse Blue 79:1 Purified Presscake, Lot Number KA0008, BRRC Sample Number 53-10. Green powder at room temperature, >97% pure.

Conclusion: In conclusion, C.I. Disperse Blue 79:1 administered to New Zealand White rabbits by gavage during gestation resulted in maternal toxicity at 300 and 600 mg/kg/day and a slight reduction in fetal body weight at 600 mg/kg/day.

There was no evidence of teratogenicity at any dose tested.

Therefore, the NOAEL for maternal toxicity was 100 mg/kg/day and for developmental toxicity was 300 mg/kg/day under the conditions of this study.

Reliability: (1) valid without restriction
GLP guideline study.

Flag: Critical study for SIDS endpoint

Reference: (3)(12)

5.10 Other Relevant Information

Type: Metabolism
Species: Rat
Year: 1991
GLP: Yes
Method: Six rats per dose level were randomly selected and placed individually into Roth-type metabolism cages for an acclimation and fasting period of 15 hours prior to dose administration. The test substance in corn oil was administered to four male and four female rats per group. The target concentrations were 500 and 50 mg/kg for the high and low dose groups, respectively. The target dose volume was 4 ml/kg of body weight and a target radioactivity of 10-15 uCi was given to each animal.

Urine and feces were collected at 6, 12, 24, 48, 72 and 96 hr post-dosing. Room air was drawn through Roth-type metabolism cages, specifically designed for collection, at a rate of approximately 500 ml/min. Expired 14-CO2 was trapped at 12, 24, 48, 72 and 96 hours post-dosing.

Ninety-six hours after administration of the dose, the animals were anesthetized and sacrificed. Selected organs were collected for analysis.

Analysis of dosing suspensions for Disperse Blue 79:1 was conducted prior to and at the conclusion of the definitive study. Analysis of urine and feces for Disperse Blue 79 and the suspected metabolite, BDNA, was also conducted using HPLC.

Result: The overall recovery for the high dose was 98.0 +/- 2.1% for the males and 92.5 +/- 2.6% for the females. For the low dose, overall recovery was 94.0 +/- 3.4% for the males and 91.7 +/- 3.3% for the females.

The majority of the radioactive dose (greater than 73%) was excreted in the feces within the first 24 hours and an additional 5-12% excreted in the second 24 hour period. Excretion of radioactivity was virtually complete by 48 hours post-dosing with less than 1% of the fecal radioactivity excreted between 48 and 96 hours.

Approximately 6% of the administered dose was excreted in urine during the 96 hour collection period, with the majority (almost 5%) excreted during the first 24 hours. Minor amounts of radioactivity were also recovered in expired carbon dioxide (0.02-0.10%), the tissues (0.03-0.14%), and in the carcas/pelt (0.00-1.40%)

Analysis of individual feces samples collected from each sex in each dose group demonstrated that the majority of detectable radioactivity was unchanged C-14 labeled DB 79:1.

An unresolved metabolite peak accounted for the balance of the radioactivity in the feces samples from all dose levels. Analysis of pooled urine samples collected at 12, 24 and 48 hour post-dosing, from each sex in each dose group, showed an unidentified metabolite effectively accounting for all of the detectable radioactivity in the urine samples from all dose levels. The suspected metabolite, 6-bromo-2,4-dinitroaniline(BDNA), did not appear in any of the urine or feces samples.

Test substance: C.I. Disperse Blue 79:1 Purified Presscake, Lot Number KA0008, BRRC Sample Number 53-10. Green powder at room temperature, >97% pure.

Conclusion: The recovery of 85 to 91% of the administered dose in the feces alone indicates that DB79:1 is probably not extensively absorbed from the GI tract of the rat following oral ingestion. It was therefore concluded by the investigators that DB79:1 is substantially cleared from the GI tract following oral doses and does not appear to be extensively metabolized.

Reliability: (1) valid without restriction

Meets generally accepted scientific method and is described in sufficient detail.

Flag: Critical study for SIDS endpoint

Reference: (3)(6)

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